International Journal of Pure and Applied Mathematics

Volume 42 No. 4 2008, 583-590

KIRKWOOD AND WIGNER DISTRIBUTION FUNCTIONS: GRAPHICAL IMAGING

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Abstract: There exists a great variety of quantum distribution functions in phase space that are widely used in many branches of quantum physics. The Kirkwood distribution function turned out to be a generating function for almost all of them. It is also known as Terletsky or Rihaczek quasi-probability. The goal of the work is to present some computer based graphical examples of Kirkwood and Wigner distribution functions for some typical systems, such as harmonic oscillator, potential and hydrogen atom, studied in physics.

AMS Subject Classification: 30-04, 60-04
Key Words: distribution functions, phase space, computer graphing

1. Introduction

In quantum physics the knowledge of distribution functions of systems is a very important task. These are functions defined in the phase space of the system, i.e. their definition area belongs to the combined configuration (position) and momentum spaces $(\vec{x}, \vec{p})$. They are considered as quasi-probabilities since some of them are not strictly non-negative functions in phase space. There exists a great variety of distribution functions for quantum systems like bosons and fermions [1]-[8], [17]-[24], [28]. It has been proved (Evtimova and Georgiev [9]) that all of them can be obtained from one basic quantum distribution function, namely the distribution function first introduced by Kirkwood [20], via the action of suitable convolution pseudo-differential operators. Thus, it turns out that it is important to know the Kirkwood distribution function

Received: August 17, 2007

for the existing different quantum systems. The basic systems regarded in quantum mechanics are: a particle in a potential well, a harmonic oscillator and hydrogen atom. The Kirkwood distribution function for them all was functionally investigated by Evtimova [10]-[13] and Georgiev, Evtimova and Dishlieva [15]. The main stream of investigations in the literature is focused on Wigner distribution function [16]-[24]. The goal for investigations of Kirkwood function is inspired by the fact that this distribution occurs in a very natural way in the quantum field invariants such as energy momentum and spin tensors of the corresponding fields (see [10], [11] for details).

The purpose of the present work is to give graphical images of these functions via the contemporary powerful computer technologies.

2. Quantum Quasi-Distributions for Harmonic Oscillator, Potential Well and Hydrogen Atom – Analytical Expressions

Here are given in explicit forms the distribution functions found in [10], [12], [13], [15] for three basic cases in quantum mechanics, namely: the functions of Wigner [28] and Kirkwood [20] for harmonic oscillator and potential well, and the Kirkwood distribution for a hydrogen atom.

The *Kirkwood distribution* in case of a *harmonic oscillator* is

$$F_{_K}^n(x,p) = \frac{1}{\pi\hbar}\mathrm{H}_n(x) Re\left(i^n \exp(ixp)\right) P_n(p), \tag{1}$$

where $H_n(.)$ is used to denote the Hermit polynomial, $x = \alpha q,\ \alpha = m\omega/\hbar$, and $P_n(p) = \sum\limits_{j=0}^{[n/2]} \frac{\partial_p^{n-2}\exp(-p^2/2)}{4^j j!(n-2j)!}$, here $[n/2]$ is the maximum of the whole part of $n/2$, $n = 1,2,3,\ldots$.

The *Wigner distribution* function of a *harmonic oscillator* has the form

$$F_W^n(q,p) = \frac{(-1)^n}{\pi\hbar}\exp\left(\frac{-2H(q,p)}{\hbar\omega}\right) L_n\left(\frac{4H(q,p)}{\hbar\omega}\right), \tag{2}$$

where L_n (.) is the Laguerre polynomial of order $n = 0,1,2,...$, and $H = \frac{p^2}{2m} + \frac{m\omega^2}{2}$ is the Hamilton function of the system.

For a one dimensional infinite *potential well* with size a one has that the *Wigner* distribution function is [15]

$$F_W^n(x,p) = \frac{-\chi_a(x)}{\pi a p}\cos\left(2k_n(x+\frac{a}{2})\right)\sin\left(2p(\frac{a}{2} - |x|)\right)$$

$$+\frac{\chi_{a(}(x)}{\pi a p}\left(\frac{\sin 2(p+k_n)(a/2-|x|)}{p+k_n}+\frac{\sin 2(p-k_n)(a/2-|x|)}{p-k_n}\right) \quad (3)$$

and the *Kirkwood* distribution function is (see [15])

$$F_K^n(x,p) = \frac{\chi_a(x) k_n \sin k_n\,(x+a/2)}{\pi a(k_n^2-p^2)}\left(\cos p(x+\frac{a}{2})-(-1)^n \cos p(x-\frac{a}{2})\right), \quad (4)$$

where $n = 1, 2, 3, \ldots$ and

$$\chi_a(x) = \begin{cases} 1, & \text{if } |x| \leq a/2\,, \\ 0, & \text{if } |x| > a/2\,. \end{cases}$$

In the case of the *hydrogen atom* it is necessary to make a generalization of the *Kirkwood* distribution for spherical coordinates both in the position and on the momentum spaces and thus applying the general theorems from [25] it was obtained in [10], [12], [13] that

$$F_K^{nlm} = C\, f(r)\, H_{\frac{3}{2}+l-m}(k_r) \frac{J_{\frac{1}{2}+l-m}(rk_r)}{(rk_r)^{\frac{1}{2}}} Y_{lm}^*(\theta,\varphi)\, Y_{lm}(k_\theta,k_\varphi)\,, \quad (5)$$

where the notations are as follows: C =const., (r,θ,ϕ) and (k_r,k_θ,k_ϕ) are the corresponding spherical coordinates into the 3-dimensional position and momentum spaces, Y_{lm} is a spherical harmonic of order $l-m$, $J_{\frac{1}{2}+l-m}(rk_r)$ is a Bessel function, $f(r)$ is connected with radial solution of Klein-Gordon equation and is equal to $f(r) = N\beta^{3/2}\,(\beta\, r)^m \Im(-n+l+1, 2l+2; \beta\, r)$, where the degenerate hyper-geometrical polynomial is taken as

$$\Im(-n+l+1, 2l+2; \beta\, r) = \sum_{s=0}^{n-l-1} (-1)^s \begin{pmatrix} n-l-1 \\ s \end{pmatrix} \frac{(2l+1)!}{(2l+s+1)!} (\beta\, r)^s,$$

the Hankel transform is

$$H_{\frac{3}{2}+l-m}(k_r) = 2\pi\, i^{m-l} \int_0^\infty f(r) \left[J_{\frac{1}{2}+l-m}(rk_r)/k_r^{\frac{1}{2}+l-m}\right] r^{\frac{3}{2}+l-m}\, dr,$$

$n = 1, 2, 3\ldots$ is the main quantum number, l is the orbital quantum number and m is the magnetic quantum number.

For the purpose of clearness we shall write down the expression of that function in the basic state of the hydrogen atom, i.e. the case with quantum numbers $n = 1$, $l = 0$, $m = 0$:

$$F_K^{100}(r,k_r)$$

$$= \frac{-8\beta^3 \exp(-{}^{\beta\, r}\!/_2)}{\sqrt{2}\pi^3(4k_r^2+\beta^2)^{3/2}} \left(\sum_{q=0}^{\infty} \frac{\Gamma(q-{}^1\!/_2)}{q!} \left(\frac{4k_r^2}{4k_r^2+\beta^2} \right)^p \right) \frac{\sin(rk_r)}{rk_r}\,, \quad (6)$$

where r and k_r are the radial variables in the position and momentum spaces respectively, $\beta = 2/r_0$, $r_0 = \hbar^2/me^2$ – the Bohr's radius and $\Gamma(.)$ is a gamma function.

3. Quantum Quasi-Distributions for Some States of Harmonic Oscillator, Potential Well and Basic State of Hydrogen Atom – Graphical Views

Plots of the two different cases of harmonic oscillator (see Figure 1 and Figure 2):

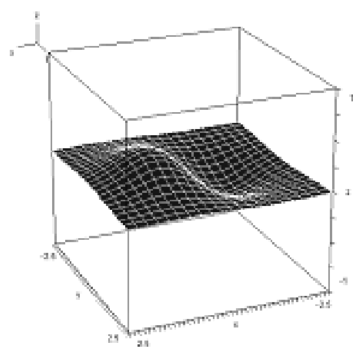

Figure 1: Real *Kirkwood* function for $n = 1$

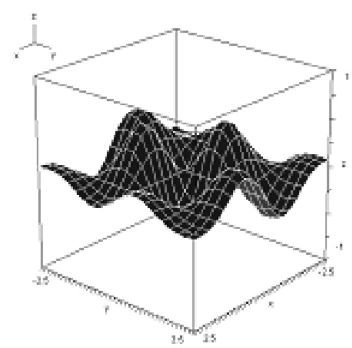

Figure 2: Real *Kirkwood* function for $n = 3$

Plots of different cases for potential well are shown on Figure 3 – Figure 6.

The graphs are drawn in a half of the potential well with a scaling multiplier that is equal to 100 in order to have a more clear vision. Potential well is taken to be ten times the Compton wavelength of the electron.

These graphs are drawn in the whole range of the potential well with a scaling multiplier that is equal to 100 in order to have a more clear vision. Potential well is taken to be ten times the Compton wavelength of the electron.

Plots of two different cases for hydrogen atom are shown on Figure 7 and Figure 8.

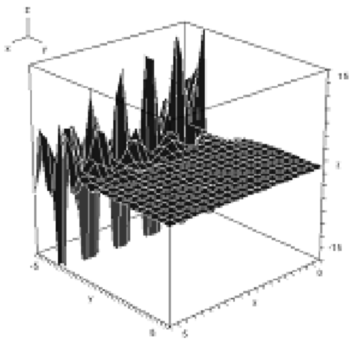

Figure 3: Real *Kirkwood* function for $n = 1$

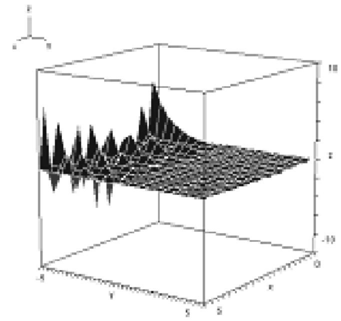

Figure 4: Real *Kirkwood* function for $n = 2$

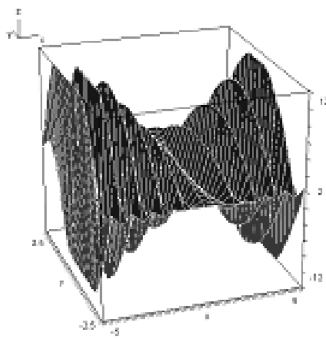

Figure 5: *Wigne*r function for $n = 1$

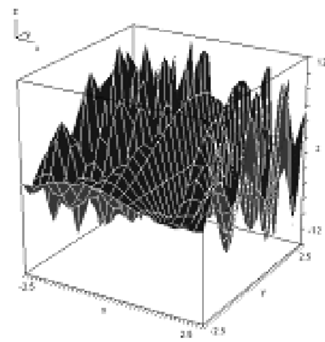

Figure 6: *Wigner* function for $n = 2$

4. Conclusions and Comments

The above shown graphical examples of views of the Wigner and Kirkwood distribution functions (for arbitrary chosen quantum numbers) bear testimony of the fact that they are not non-negative everywhere over their definition areas. Because of the existence of some negative values in the quantum distribution functions they are not considered as true probability distributions in classical meaning and that is why they are called quasi-distributions. Nevertheless they have been applied successfully in many branches of the quantum physics, as they are used as tools of finding average (measurable) values for many quantities as positions, momentums and energies of particles and systems. Since the quantum numbers usually range from one to infinity it is neither possible nor necessary

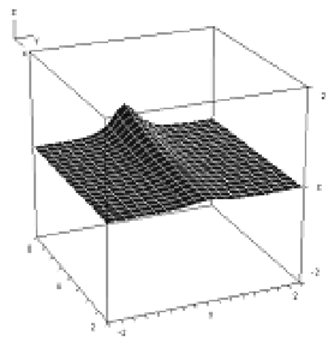

Figure 7: Real *Kirkwood* distribution function for the principal state ($n = 1,\ l = m = 0$) of the hydrogen atom in dimensionless position-momentum (x, y) coordinates. Actually, $x = 1$ is considered to represent the Bohr radius (first orbital) and $y = \beta k_r$

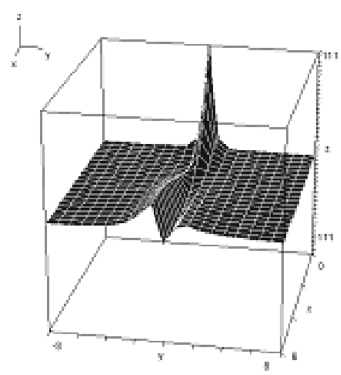

Figure 8: Real *Kirkwood* distribution function for the first exited state ($n = 2,\ l = 1,\ m = 0$) of the hydrogen atom in dimensionless position-momentum (x, y) coordinates. Actually, x = 1 is considered to represent the Bohr radius (first orbital) and $y = \beta k_r$. This graph is drawn again with a scaling multiplier that is equal to 100 in order to have a more clear vision.

to look for more examples.

As it is known from the literature there is no negative values for the basic state of harmonic oscillator if the distribution is calculated via Wigner function, but Kirkwood function do have some negative values in the same situation. In the case of quantum numbers $n > 1$ both Wigner and Kirkwood functions do possess negative values. It is clear from the graphs that there exist definite regions of positive-ness and negative-ness of these functions. They are separated by the lines of nullifying the corresponding distribution functions (1) – (6). On Figure 7 the graph of the real Kirkwood distribution function (6) in (x, y) - coordinates is given, where the values of x are taken to be only positive since it represents the radial variable in (5). The maximal value of this function is at the point $(x, y) = (0{,}0)$ $(y = \beta k_r)$and it is maxF_K = 0,51681. The minimal value is equal to - $4{,}52915.10^{-5}$ and it is at the point (x, y) = (1,92; 2,16). The fact that Kirkwood function has a maximum at the origin of the coordinate system is connected with the corresponding representations of the position and momentum wave functions. Since the wave vectors (momentums) of the constituents of the electron are uniformly distributed in all directions the result is that they compensate at the center of the atom. So the integration of function (5) over the momentums (wave numbers) gives the right quantum-mechanical distribution in the space.

The stress of the investigation is put on the Kirkwood distribution function since as it was proved in [9] this function is a critical point (bears extremum properties) of the entropy-like functional in the space of all quantum distribution functions.

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